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# Origin of fluorine/sulfur *gauche* effect of β-fluorinated thiol, sulfoxide, sulfone and thionium ion

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## *Supporting Information*

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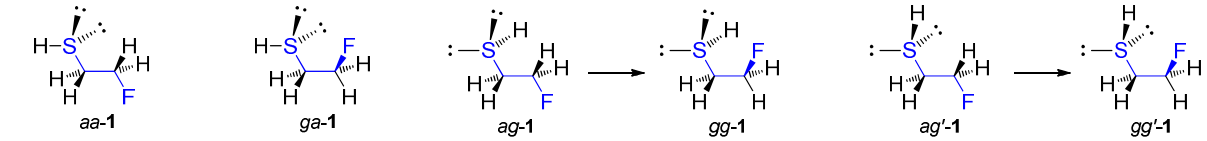
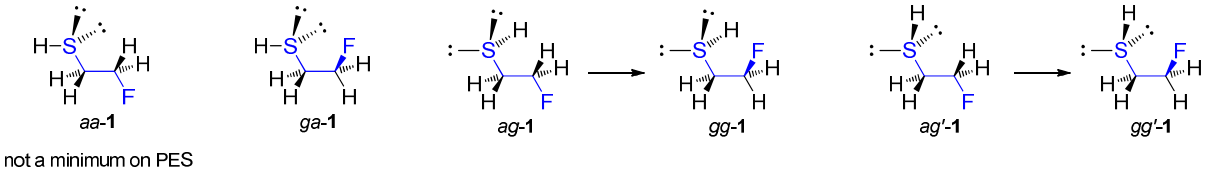
**Table S1.** Calculated relative electronic energies ΔE, enthalpies ΔH and free energies ΔG of four conformers of **1** and energy changes (in bold) occuring upon conformational isomerization (MP2/6-311++G(d,p) regular, B3LYP/6-311++G(d,p) italic). Values are in kcal/mol.




| conformation | gas-phase | | | in $CH_2Cl_2$ | | | in $Me_2CO$ | | | in $H_2O$ | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | ΔE | ΔH | ΔG | ΔE | ΔH | ΔG | ΔE | ΔH | ΔG | ΔE | ΔH | ΔG |
| *ag/g′*-**1** | 0.24 | 0.29 | 0.18 | 0.11 | 0.22 | 0.13 | 0.11 | 0.22 | 0.18 | 0.10 | 0.23 | 0.21 |
| | *0.18* | *0.27* | *0.10* | *0.18* | *0.28* | *0.17* | *0.19* | *0.28* | *0.16* | *0.20* | *0.28* | *0.15* |
| *ga*-**1** | 2.29 | 2.28 | 1.90 | 1.58 | 1.62 | 1.31 | 1.47 | 1.51 | 1.20 | 1.39 | 1.44 | 1.13 |
| | *2.25* | *2.23* | *1.72* | *1.53* | *1.55* | *1.20* | *1.42* | *1.42* | *1.01* | *1.34* | *1.34* | *0.87* |
| *gg*-**1** | 1.85 | 1.77 | 1.57 | 0.83 | 0.82 | 0.74 | 0.67 | 0.67 | 0.60 | 0.57 | 0.57 | 0.52 |
| | *1.69* | *1.63* | *1.38* | *0.72* | *0.73* | *0.66* | *0.56* | *0.57* | *0.52* | *0.46* | *0.47* | *0.42* |
| *gg′*-**1** | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| | *0.00* | *0.00* | *0.00* | *0.00* | *0.00* | *0.00* | *0.00* | *0.00* | *0.00* | *0.00* | *0.00* | *0.00* |
| *ag*-**1** → *gg*-**1** | **1.61** | **1.48** | **1.39** | **0.71** | **0.60** | **0.60** | **0.57** | **0.44** | **0.43** | **0.47** | **0.34** | **0.31** |
| | ***1.51*** | ***1.37*** | ***1.28*** | ***0.54*** | ***0.45*** | ***0.49*** | ***0.37*** | ***0.29*** | ***0.36*** | ***0.27*** | ***0.19*** | ***0.28*** |
| *ag′*-**1** → *gg′*-**1** | **-0.24** | **-0.29** | **-0.18** | **-0.11** | **-0.22** | **-0.13** | **-0.11** | **-0.22** | **-0.18** | **-0.10** | **-0.23** | **-0.21** |
| | ***-0.18*** | ***-0.27*** | ***-0.10*** | ***-0.18*** | ***-0.28*** | ***-0.17*** | ***-0.19*** | ***-0.28*** | ***-0.16*** | ***-0.20*** | ***-0.28*** | ***-0.15*** |

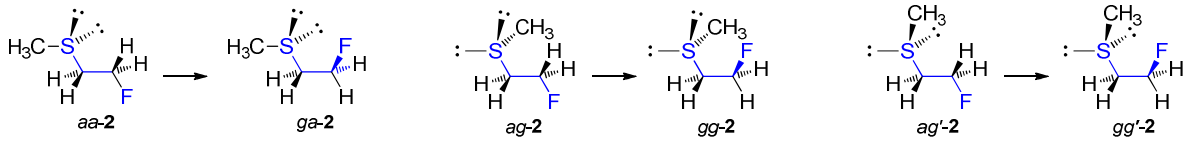
**Table S2.** Contribution of various energy components to the total binding interactions between two $FCH_2\cdot$ and $\cdot CH_2SH$ fragments and energy changes (ΔΔE values, in bold) occuring upon conformational isomerization.[a] EDA results for 2-fluoroethanol (FE) are included, too.[b] Values are in kcal/mol.




| conformation | $\Delta E_{tot}$ **$\Delta E_{iso}$** | $\Delta E_{def}$ **$\Delta\Delta E_{def}$** | $\Delta E_{int}$ **$\Delta\Delta E_{int}$** | $\Delta E_{elstat}$ **$\Delta\Delta E_{elstat}$** | $\Delta E_{ex+rep}$ **$\Delta\Delta E_{ex+rep}$** | $\Delta E_{oi}$ **$\Delta\Delta E_{oi}$** | $\Delta E_{disp}$ **$\Delta\Delta E_{disp}$** |
|---|---|---|---|---|---|---|---|
| *ag/g′*-**1** | -95.12 | 13.33 | -108.45 | -154.61 | 234.40 | -159.04 | -29.20 |
| *ga*-**1** | -93.07 | 18.71 | -111.78 | -149.93 | 226.12 | -156.79 | -31.18 |
| *gg*-**1** | -93.50 | 13.41 | -106.91 | -153.39 | 234.46 | -158.96 | -29.02 |
| *gg′*-**1** | -95.37 | 13.86 | -109.23 | -155.64 | 235.25 | -159.46 | -29.38 |
| *ag*-**1** → *gg*-**1** | **1.61** | **0.07** | **1.54** | **1.22** | **0.06** | **0.08** | **0.18** |
| *ag′*-**1** → *gg′*-**1** | **-0.24** | **0.54** | **-0.78** | **-1.03** (63%) | **0.85** | **-0.42** (26%) | **-0.18** (11%) |
| *ag*-FE → *gg*-FE | **0.09** | **0.75** | **-0.66** | **-1.28** | **3.86** | **-2.55** | **-0.69** |
| *ag′*-FE → *gg′*-FE | **-2.54** | **0.57** | **-3.11** | **-5.34** | **5.77** | **-3.03** | **-0.51** |

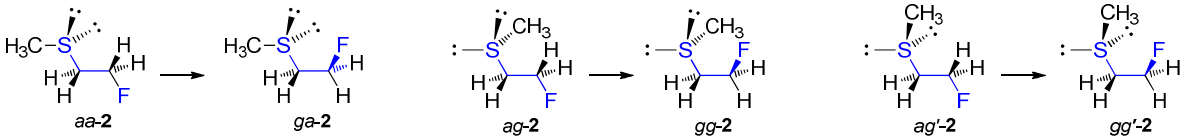
[a] $\Delta E_{tot}$ = total binding energy between two radical fragments, $\Delta E_{def}$ = deformation energy, $\Delta E_{int}$ = interaction energy, $\Delta E_{elstat}$ = electrostatic energy, $\Delta E_{ex+rep}$ = exchange repulsion energy, $\Delta E_{oi}$ = orbital interaction energy, $\Delta E_{disp}$ = dispersion energy, $\Delta E_{iso}$ = isomerization energy, ΔΔE values represent individual energy changes upon conformational isomerization. Values in parentheses are percentage contribution to all attractive interactions. [b] From ref. 8e.

**Table S3.** Calculated relative electronic energies ΔE, enthalpies ΔH and free energies ΔG of five conformers of **2** and energy changes (in bold) occuring upon conformational isomerization (MP2/6-311++G(d,p)). Values are in kcal/mol.




| conformation | gas-phase | | | in $CH_2Cl_2$ | | | in $Me_2CO$ | | | in $H_2O$ | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | ΔE | ΔH | ΔG | ΔE | ΔH | ΔG | ΔE | ΔH | ΔG | ΔE | ΔH | ΔG |
| *aa*-**2** | 1.18 | 1.28 | 0.94 | 1.34 | 1.42 | 1.17 | 1.37 | 1.44 | 1.17 | 1.38 | 1.45 | 1.17 |
| *ag/g′*-**2** | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| *ga*-**2** | 1.68 | 1.65 | 1.48 | 1.07 | 1.01 | 0.92 | 0.95 | 0.89 | 0.77 | 0.87 | 0.80 | 0.67 |
| *gg*-**2** | 1.32 | 1.17 | 1.14 | 0.44 | 0.35 | 0.49 | 0.29 | 0.19 | 0.31 | 0.19 | 0.09 | 0.20 |
| *gg′*-**2** | 0.20 | 0.08 | 0.21 | 0.31 | 0.22 | 0.43 | 0.30 | 0.21 | 0.41 | 0.30 | 0.20 | 0.39 |
| *aa*-**2** → *ga*-**2** | **0.50** | **0.37** | **0.54** | **-0.28** | **-0.41** | **-0.25** | **-0.42** | **-0.56** | **-0.40** | **-0.52** | **-0.65** | **-0.50** |
| *ag*-**2** → *gg*-**2** | **1.32** | **1.17** | **1.14** | **0.44** | **0.35** | **0.49** | **0.29** | **0.19** | **0.31** | **0.19** | **0.09** | **0.20** |
| *ag′*-**2** → *gg′*-**2** | **0.20** | **0.08** | **0.21** | **0.31** | **0.22** | **0.43** | **0.30** | **0.21** | **0.41** | **0.30** | **0.20** | **0.39** |

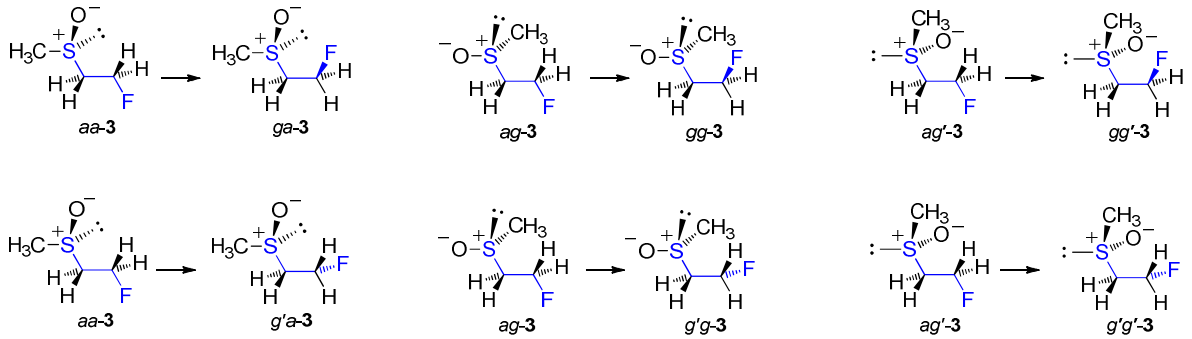
**Table S4.** Contribution of various energy components to the total binding interactions between two $FCH_2\cdot$ and $\cdot CH_2SCH_3$ fragments and energy changes (ΔΔE values, in bold) occuring upon conformational isomerization.[a] Values are in kcal/mol.




| conformation | $\Delta E_{tot}$ | $\Delta E_{def}$ | $\Delta E_{int}$ | $\Delta E_{elstat}$ | $\Delta E_{ex+rep}$ | $\Delta E_{oi}$ | $\Delta E_{disp}$ |
|---|---|---|---|---|---|---|---|
| | $\mathbf{\Delta E_{iso}}$ | $\mathbf{\Delta\Delta E_{def}}$ | $\mathbf{\Delta\Delta E_{int}}$ | $\mathbf{\Delta\Delta E_{elstat}}$ | $\mathbf{\Delta\Delta E_{ex+rep}}$ | $\mathbf{\Delta\Delta E_{oi}}$ | $\mathbf{\Delta\Delta E_{disp}}$ |
| *aa*-**2** | -92.41 | 20.25 | -112.66 | -148.44 | 221.14 | -154.55 | -30.81 |
| *ag/g′*-**2** | -93.59 | 13.37 | -106.96 | -157.05 | 238.86 | -160.13 | -28.64 |
| *ga*-**2** | -91.92 | 20.48 | -112.40 | -148.38 | 222.60 | -155.47 | -31.15 |
| *gg*-**2** | -92.27 | 13.60 | -105.87 | -155.49 | 238.15 | -159.81 | -28.72 |
| *gg′*-**2** | -93.40 | 13.58 | -106.98 | -158.19 | 240.35 | -160.74 | -28.40 |
| *aa*-**2** → *ga*-**2** | **0.50** | **0.24** | **0.26** | **0.06** | **1.46** | **-0.92** | **-0.34** |
| *ag*-**2** → *gg*-**2** | **1.32** | **0.23** | **1.09** | **1.56** | **-0.71** | **0.32** | **-0.08** |
| *ag′*-**2** → *gg′*-**2** | **0.20** | **0.22** | **-0.02** | **-1.14** | **1.49** | **-0.61** | **0.24** |

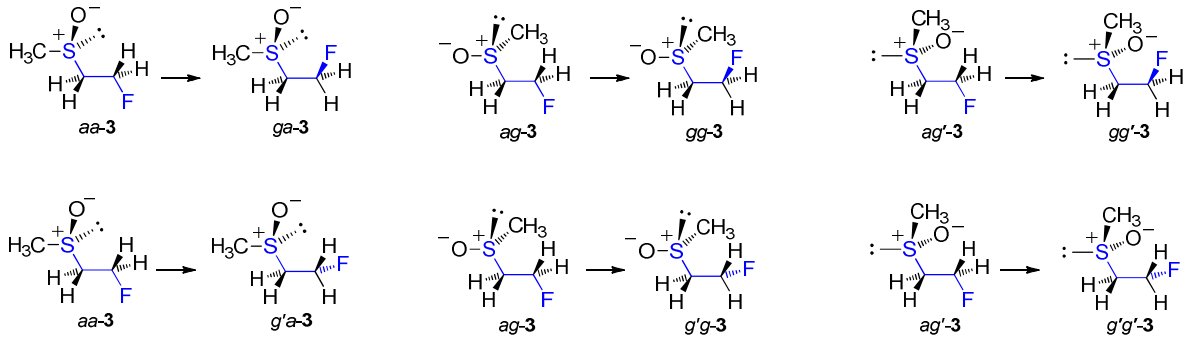
[a] Labeling of various energy terms is the same as in Table S2. Values in parentheses are percentage contribution to all attractive interactions.

**Table S5.** Calculated relative electronic energies ΔE, enthalpies ΔH and free energies ΔG of nine conformers of **3** and energy changes (in bold) occuring upon conformational isomerization (MP2/6-311++G(d,p)). Values are in kcal/mol.




| conformation | gas-phase | | | in $CH_2Cl_2$ | | | in $Me_2CO$ | | | in $H_2O$ | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | ΔE | ΔH | ΔG | ΔE | ΔH | ΔG | ΔE | ΔH | ΔG | ΔE | ΔH | ΔG |
| *aa*-**3** | 1.29 | 1.35 | 0.96 | 1.48 | 1.48 | 1.14 | 1.43 | 1.53 | 1.20 | 1.48 | 1.57 | 1.23 |
| *ag*-**3** | 2.93 | 3.05 | 2.75 | 2.56 | 2.56 | 2.60 | 2.33 | 2.54 | 2.59 | 2.32 | 2.53 | 2.58 |
| *ag′*-**3** | 1.95 | 2.08 | 1.69 | 2.15 | 2.15 | 2.10 | 1.96 | 2.20 | 2.19 | 1.99 | 2.24 | 2.27 |
| *ga*-**3** | 3.81 | 3.80 | 3.44 | 1.90 | 1.90 | 1.94 | 1.96 | 1.60 | 1.62 | 1.41 | 1.40 | 1.39 |
| *gg*-**3** | 2.23 | 2.27 | 2.06 | 1.54 | 1.54 | 1.38 | 1.42 | 1.51 | 1.41 | 1.39 | 1.47 | 1.36 |
| *gg′*-**3** | 0.00 | 0.00 | 0.00 | 0.59 | 0.59 | 0.70 | 0.58 | 0.70 | 0.80 | 0.65 | 0.76 | 0.85 |
| *g′a*-**3** | 0.29 | 0.24 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| *g′g*-**3** | 1.14 | 1.11 | 0.91 | 1.08 | 1.08 | 0.97 | 1.11 | 1.15 | 1.05 | 1.17 | 1.20 | 1.10 |
| *g′g′*-**3** | 4.75 | 4.61 | 4.10 | 3.13 | 3.13 | 3.30 | 2.85 | 2.87 | 3.02 | 2.67 | 2.70 | 2.80 |
| *aa*-**3** → *ga*-**3** | **2.52** | **2.45** | **2.48** | **0.43** | **0.43** | **0.80** | **0.18** | **0.07** | **0.42** | **-0.06** | **-0.17** | **0.16** |
| *aa*-**3** → *g′a*-**3** | **-1.00** | **-1.11** | **-0.95** | **-1.48** | **-1.48** | **-1.14** | **-1.43** | **-1.53** | **-1.20** | **-1.48** | **-1.57** | **-1.23** |
| *ag*-**3** → *gg*-**3** | **-0.70** | **-0.78** | **-0.69** | **-1.01** | **-1.01** | **-1.22** | **-0.92** | **-1.03** | **-1.18** | **-0.93** | **-1.05** | **-1.22** |
| *ag*-**3** → *g′g*-**3** | **-1.79** | **-1.94** | **-1.84** | **-1.48** | **-1.48** | **-1.63** | **-1.22** | **-1.38** | **-1.54** | **-1.15** | **-1.32** | **-1.48** |
| *ag′*-**3** → *gg′*-**3** | **-1.95** | **-2.08** | **-1.69** | **-1.57** | **-1.57** | **-1.39** | **-1.38** | **-1.50** | **-1.39** | **-1.33** | **-1.47** | **-1.42** |
| *ag′*-**3**→ *g′g′*-**3** | **2.80** | **2.53** | **2.41** | **0.98** | **0.98** | **1.20** | **0.89** | **0.67** | **0.84** | **0.68** | **0.46** | **0.52** |

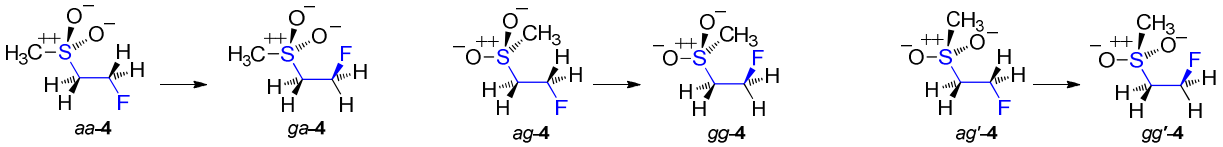
**Table S6.** Contribution of various energy components to the total binding interactions between two $FCH_2$· and ·$CH_2SOCH_3$ fragmentls and energy changes (ΔΔE values, in bold) occuring upon conformational isomerization.[a] Values are in kcal/mol.




| conformation | $\Delta E_{tot}$ **$\Delta E_{iso}$** | $\Delta E_{def}$ **$\Delta\Delta E_{def}$** | $\Delta E_{int}$ **$\Delta\Delta E_{int}$** | $\Delta E_{elstat}$ **$\Delta\Delta E_{elstat}$** | $\Delta E_{ex+rep}$ **$\Delta\Delta E_{ex+rep}$** | $\Delta E_{oi}$ **$\Delta\Delta E_{oi}$** | $\Delta E_{disp}$ **$\Delta\Delta E_{disp}$** |
|---|---|---|---|---|---|---|---|
| *aa*-**3** | -99.36 | 15.42 | -114.78 | -144.94 | 214.69 | -153.47 | -31.06 |
| *ag*-**3** | -97.72 | 14.30 | -112.02 | -144.49 | 217.66 | -154.70 | -30.49 |
| *ag′*-**3** | -98.70 | 13.83 | -112.53 | -146.92 | 220.52 | -155.82 | -30.31 |
| *ga*-**3** | -96.83 | 15.34 | -112.17 | -144.62 | 218.73 | -154.92 | -31.36 |
| *gg*-**3** | -98.42 | 14.74 | -113.16 | -146.85 | 219.82 | -155.87 | -30.26 |
| *gg′*-**3** | -100.65 | 14.46 | -115.11 | -150.53 | 223.69 | -157.59 | -30.68 |
| *g′a*-**3** | -100.35 | 15.40 | -115.75 | -147.30 | 218.25 | -155.33 | -31.37 |
| *g′g*-**3** | -99.50 | 15.10 | -114.60 | -148.99 | 220.40 | -155.96 | -30.05 |
| *g′g′*-**3** | -95.89 | 15.69 | -111.58 | -141.99 | 215.34 | -153.70 | -31.23 |
| *aa*-**3** → *ga*-**3** | **2.52** | **-0.09** | **2.61** | **0.32** | **4.04** | **-1.45** | **-0.30** |
| *aa*-**3** → *g′a*-**3** | **-1.00** | **-0.03** | **-0.97** | **-2.36** (52%) | **3.56** | **-1.86** (41%) | **-0.31** (7%) |
| *ag*-**3** → *gg*-**3** | **-0.70** | **0.44** | **-1.14** | **-2.36** (67%) | **2.16** | **-1.17** (33%) | **0.23** |
| *ag*-**3** → *g′g*-**3** | **-1.79** | **0.79** | **-2.58** | **-4.50** (78%) | **2.74** | **-1.26** (22%) | **0.44** |
| *ag′*-**3** → *gg′*-**3** | **-1.95** | **0.63** | **-2.58** | **-3.61** (63%) | **3.17** | **-1.77** (31%) | **-0.38** (6%) |
| *ag′*-**3**→ *g′g′*-**3** | **2.80** | **1.85** | **0.95** | **4.93** | **-5.18** | **2.12** | **-0.92** |

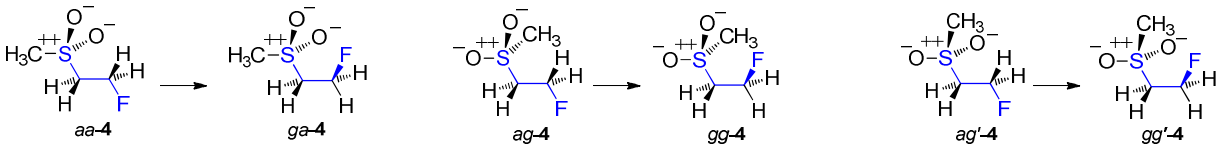
[a] Labeling of various energy terms is the same as in Table S2. Values in parentheses are percentage contribution to all attractive interactions.

**Table S7.** Calculated relative electronic energies ΔE, enthalpies ΔH and free energies ΔG of five conformers of **4** and energy changes (in bold) occuring upon conformational isomerization (MP2/6-311++G(d,p)). Values are in kcal/mol.




| conformation | gas-phase | | | in $CH_2Cl_2$ | | | in $Me_2CO$ | | | in $H_2O$ | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | ΔE | ΔH | ΔG | ΔE | ΔH | ΔG | ΔE | ΔH | ΔG | ΔE | ΔH | ΔG |
| *aa*-**4** | 2.13 | 2.36 | 1.63 | 2.15 | 2.21 | 1.14 | 2.13 | 2.21 | 1.33 | 2.11 | 2.21 | 1.49 |
| *ag/g′*-**4** | 2.34 | 2.47 | 2.16 | 2.04 | 2.15 | 1.95 | 1.97 | 2.09 | 1.84 | 1.94 | 2.05 | 1.74 |
| *ga*-**4** | 3.46 | 3.54 | 3.27 | 1.70 | 1.71 | 1.57 | 1.34 | 1.36 | 1.27 | 1.11 | 1.13 | 1.03 |
| *gg*-**4** | 4.59 | 4.52 | 4.47 | 2.55 | 2.66 | 2.76 | 2.05 | 1.95 | 1.75 | 1.80 | 1.72 | 1.47 |
| *gg′*-**4** | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| *aa*-**4** → *ga*-**4** | **1.33** | **1.18** | **1.64** | **-0.45** | **-0.51** | **0.44** | **-0.78** | **-0.84** | **-0.06** | **-1.00** | **-1.08** | **-0.45** |
| *ag*-**4** → *gg*-**4** | **2.25** | **2.05** | **2.31** | **0.51** | **0.51** | **0.81** | **0.07** | **-0.13** | **-0.08** | **-0.13** | **-0.33** | **-0.27** |
| *ag′*-**4** → *gg′*-**4** | **-2.34** | **-2.47** | **-2.16** | **-2.04** | **-2.15** | **-1.95** | **-1.97** | **-2.09** | **-1.84** | **-1.94** | **-2.05** | **-1.74** |

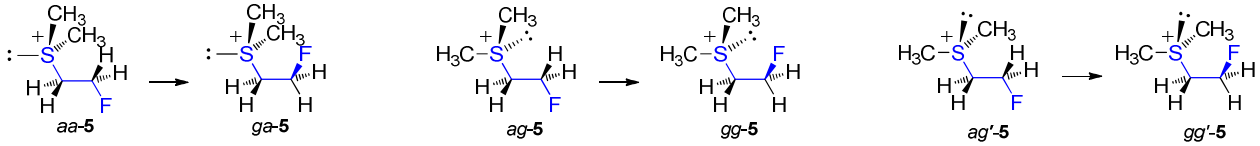
**Table S8.** Contribution of various energy components to the total binding interactions between two $FCH_2\cdot$ and $\cdot CH_2SO_2CH_3$ fragments and energy changes (ΔΔE values, in bold) occuring upon conformational isomerization.[a] Values are in kcal/mol.




| conformation | $\Delta E_{tot}$ **$\Delta E_{iso}$** | $\Delta E_{def}$ **$\Delta\Delta E_{def}$** | $\Delta E_{int}$ **$\Delta\Delta E_{int}$** | $\Delta E_{elstat}$ **$\Delta\Delta E_{elstat}$** | $\Delta E_{ex+rep}$ **$\Delta\Delta E_{ex+rep}$** | $\Delta E_{oi}$ **$\Delta\Delta E_{oi}$** | $\Delta E_{disp}$ **$\Delta\Delta E_{disp}$** |
|---|---|---|---|---|---|---|---|
| *aa*-**4** | -100.95 | 13.97 | -114.92 | -139.54 | 207.51 | -152.08 | -30.81 |
| *ag/g′*-**4** | -100.74 | 13.07 | -113.81 | -141.24 | 210.96 | -153.33 | -30.20 |
| *ga*-**4** | -99.62 | 14.58 | -114.20 | -139.36 | 210.87 | -154.16 | -31.55 |
| *gg*-**4** | -98.49 | 13.92 | -112.41 | -140.88 | 214.04 | -154.15 | -31.42 |
| *gg′*-**4** | -103.07 | 13.27 | -116.34 | -146.37 | 216.19 | -156.15 | -30.01 |
| *aa*-**4** → *ga*-**4** | **1.33** | **0.61** | **0.72** | **0.18** | **3.36** | **-2.08** | **-0.74** |
| *ag*-**4** → *gg*-**4** | **2.25** | **0.85** | **1.40** | **0.36** | **3.08** | **-0.82** | **-1.22** |
| *ag′*-**4** → *gg′*-**4** | **-2.34** | **0.19** | **-2.53** | **-5.13** (65%) | **5.23** | **-2.82** (35%) | **0.19** |

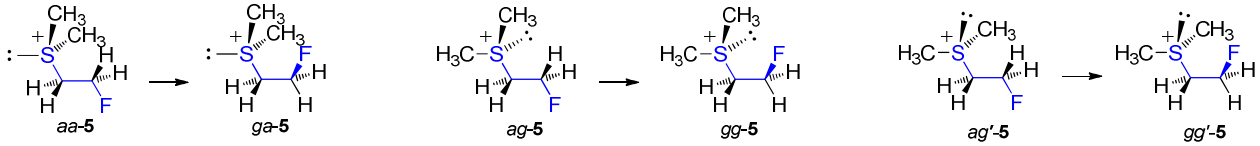
[a] Labeling of various energy terms is the same as in Table S2. Values in parentheses are percentage contribution to all attractive interactions.

**Table S9.** Calculated relative electronic energies ΔE, enthalpies ΔH and free energies ΔG of five conformers of **5** and energy changes (in bold) occuring upon conformational isomerization (MP2/6-311++G(d,p) regular, B3LYP/6-311++G(d,p) italic). Values are in kcal/mol.




| conformation | gas-phase | | | in $CH_2Cl_2$ | | | in $Me_2CO$ | | | in $H_2O$ | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | ΔE | ΔH | ΔG | ΔE | ΔH | ΔG | ΔE | ΔH | ΔG | ΔE | ΔH | ΔG |
| *aa*-**5** | 6.05 | 6.09 | 5.62 | 3.48 | 3.25 | 3.95 | 3.25 | 2.85 | 3.29 | 3.11 | 2.56 | 2.90 |
| | *5.96* | *6.05* | *5.61* | *3.46* | *3.62* | *2.35* | *3.21* | *3.32* | *2.16* | *3.07* | *3.12* | *1.78* |
| *ag/g′*-**5** | 5.03 | 5.01 | 4.50 | 2.53 | 2.79 | 2.86 | 2.31 | 2.45 | 2.25 | 2.18 | 2.24 | 1.95 |
| | *4.88* | *4.92* | *4.35* | *2.48* | *2.73* | *2.44* | *2.23* | *2.49* | *2.37* | *2.08* | *2.34* | *2.41* |
| *ga*-**5** | 0.75 | 0.73 | 1.12 | 0.92 | 0.96 | 1.25 | 0.97 | 1.02 | 1.29 | 1.01 | 1.06 | 1.47 |
| | *0.84* | *0.89* | *1.02* | *1.06* | *1.12* | *1.01* | *1.08* | *1.13* | *1.09* | *1.10* | *1.09* | *0.91* |
| *gg*-**5** | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.11 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| | *0.00* | *0.00* | *0.00* | *0.00* | *0.00* | *0.00* | *0.00* | *0.00* | *0.00* | *0.00* | *0.00* | *0.00* |
| *gg′*-**5** | 1.61 | 1.65 | 1.52 | 0.65 | 0.51 | 0.00 | 0.53 | 0.48 | 0.26 | 0.47 | 0.38 | 0.19 |
| | *1.90* | *1.90* | *1.61* | *0.57* | *0.71* | *0.55* | *0.45* | *0.56* | *0.49* | *0.38* | *0.46* | *0.48* |
| *aa*-**5** → *ga*-**5** | **-5.30** | **-5.36** | **-4.50** | **-2.57** | **-2.29** | **-2.69** | **-2.28** | **-1.84** | **-2.00** | **-2.10** | **-1.50** | **-1.43** |
| | ***-5.12*** | ***-5.16*** | ***-4.59*** | ***-2.40*** | ***-2.50*** | ***-1.34*** | ***-2.13*** | ***-2.19*** | ***-1.07*** | ***-1.97*** | ***-2.03*** | ***-0.87*** |
| *ag*-**5** → *gg*-**5** | **-5.03** | **-5.01** | **-4.50** | **-2.53** | **-2.79** | **-2.75** | **-2.31** | **-2.45** | **-2.25** | **-2.18** | **-2.24** | **-1.95** |
| | ***-4.88*** | ***-4.92*** | ***-4.35*** | ***-2.48*** | ***-2.73*** | ***-2.44*** | ***-2.23*** | ***-2.49*** | ***-2.37*** | ***-2.08*** | ***-2.34*** | ***-2.41*** |
| *ag′*-**5** → *gg′*-**5** | **-3.42** | **-3.36** | **-2.98** | **-1.88** | **-2.28** | **-2.86** | **-1.78** | **-1.97** | **-1.99** | **-1.71** | **-1.86** | **-1.77** |
| | ***-2.98*** | ***-3.02*** | ***-2.74*** | ***-1.91*** | ***-2.02*** | ***-1.89*** | ***-1.79*** | ***-1.93*** | ***-1.89*** | ***-1.70*** | ***-1.88*** | ***-1.92*** |

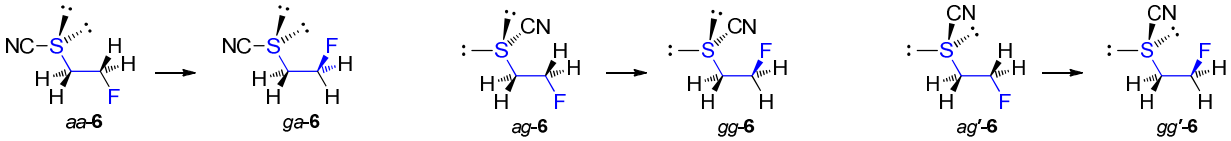
**Table S10.** Contribution of various energy components to the total binding interactions between two $FCH_2\cdot$ and $\cdot CH_2S(CH_3)_2^+$ fragments and energy changes ($\Delta\Delta E$ values, in bold) occuring upon conformational isomerization.[a] Values are in kcal/mol.




| conformation | $\Delta E_{tot}$ **$\Delta E_{iso}$** | $\Delta E_{def}$ **$\Delta\Delta E_{def}$** | $\Delta E_{int}$ **$\Delta\Delta E_{int}$** | $\Delta E_{elstat}$ **$\Delta\Delta E_{elstat}$** | $\Delta E_{ex+rep}$ **$\Delta\Delta E_{ex+rep}$** | $\Delta E_{oi}$ **$\Delta\Delta E_{oi}$** | $\Delta E_{disp}$ **$\Delta\Delta E_{disp}$** |
|---|---|---|---|---|---|---|---|
| *aa*-**5** | -95.58 | 13.06 | -108.64 | -132.10 | 207.69 | -152.81 | -31.42 |
| *ag*/*g′*-**5** | -96.61 | 14.63 | -111.24 | -130.67 | 202.32 | -151.29 | -31.60 |
| *ga*-**5** | -100.90 | 14.41 | -115.31 | -140.93 | 212.79 | -155.79 | -31.38 |
| *gg*-**5** | -101.65 | 15.16 | -116.81 | -139.70 | 209.19 | -154.94 | -31.36 |
| *gg′*-**5** | -100.03 | 15.24 | -115.27 | -135.99 | 206.63 | -153.82 | -32.09 |
| *aa*-**5** → *ga*-**5** | **-5.30** | **1.37** | **-6.67** | **-8.83** (75%) | **5.10** | **-2.98** (25%) | **0.04** |
| *ag*-**5** → *gg*-**5** | **-5.03** | **0.54** | **-5.57** | **-9.03** (71%) | **6.87** | **-3.65** (29%) | **0.24** |
| *ag′*-**5** → *gg′*-**5** | **-3.42** | **0.61** | **-4.03** | **-5.32** (64%) | **4.31** | **-2.53** (30%) | **-0.49** (6%) |

[a] Labeling of various energy terms is the same as in Table S2. Values in parentheses are percentage contribution to all attractive interactions.

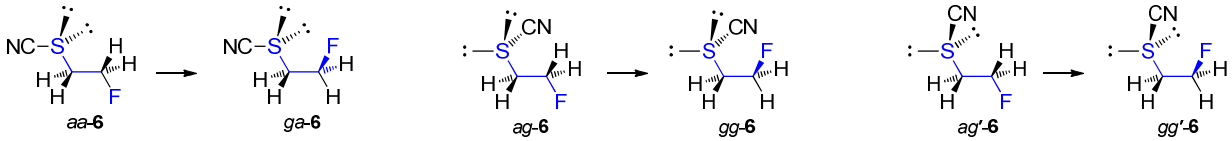
**Table S11.** Calculated relative electronic energies ΔE, enthalpies ΔH and free energies ΔG of five conformers of **6** and energy changes (in bold) occuring upon conformational isomerization (MP2/6-311++G(d,p) regular, B3LYP/6-311++G(d,p) italic). Values are in kcal/mol.




| conformation | gas-phase | | | in $CH_2Cl_2$ | | | in $Me_2CO$ | | | in $H_2O$ | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | ΔE | ΔH | ΔG | ΔE | ΔH | ΔG | ΔE | ΔH | ΔG | ΔE | ΔH | ΔG |
| *aa*-**6**[a] | 2.51 | 2.61 | 2.07 | 2.67 | 2.86 | 2.44 | / | / | / | / | / | / |
| | *2.02* | *2.17* | *0.86* | *1.81* | *1.86* | *1.34* | *1.79* | *1.85* | *1.44* | *1.78* | *1.84* | *1.49* |
| *ag/g′*-**6** | 0.00 | 0.00 | 0.00 | 0.35 | 0.45 | 0.39 | 0.41 | 0.52 | 0.46 | 0.46 | 0.56 | 0.51 |
| | *0.01* | *0.12* | *0.09* | *0.57* | *0.70* | *0.73* | *0.64* | *0.77* | *0.80* | *0.68* | *0.82* | *0.84* |
| *ga*-**6** | 1.50 | 1.50 | 1.22 | 1.39 | 1.44 | 1.03 | 1.40 | 1.46 | 1.09 | 1.41 | 1.47 | 1.12 |
| | *0.96* | *0.99* | *0.60* | *0.95* | *0.99* | *0.63* | *0.95* | *1.00* | *0.63* | *0.96* | *1.00* | *0.60* |
| *gg*-**6** | 0.16 | 0.06 | 0.07 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| | *0.00* | *0.00* | *0.00* | *0.00* | *0.00* | *0.00* | *0.00* | *0.00* | *0.00* | *0.00* | *0.00* | *0.00* |
| *gg′*-**6** | 1.66 | 1.50 | 1.51 | 0.45 | 0.41 | 0.41 | 0.29 | 0.26 | 0.28 | 0.19 | 0.16 | 0.20 |
| | *1.46* | *1.43* | *1.39* | *0.44* | *0.43* | *0.39* | *0.27* | *0.27* | *0.34* | *0.16* | *0.17* | *0.28* |
| *aa*-**6** → *ga*-**6** | **-1.01** | **-1.11** | **-0.85** | **-1.28** | **-1.42** | **-1.41** | / | / | / | / | / | / |
| | ***-1.06*** | ***-1.19*** | ***-0.25*** | ***-1.43*** | ***-1.56*** | ***-1.44*** | ***-1.48*** | ***-1.62*** | ***-1.61*** | ***-1.51*** | ***-1.66*** | ***-1.74*** |
| *ag*-**6** → *gg*-**6** | **0.16** | **0.06** | **0.07** | **-0.35** | **-0.45** | **-0.39** | **-0.41** | **-0.52** | **-0.46** | **-0.46** | **-0.56** | **-0.51** |
| | ***-0.01*** | ***-0.12*** | ***-0.09*** | ***-0.57*** | ***-0.70*** | ***-0.73*** | ***-0.64*** | ***-0.77*** | ***-0.80*** | ***-0.68*** | ***-0.82*** | ***-0.84*** |
| *ag′*-**6** → *gg′*-**6** | **1.66** | **1.50** | **1.51** | **0.10** | **-0.04** | **0.03** | **-0.12** | **-0.26** | **-0.19** | **-0.26** | **-0.40** | **-0.32** |
| | ***1.46*** | ***1.30*** | ***1.30*** | ***-0.13*** | ***-0.27*** | ***-0.35*** | ***-0.37*** | ***-0.50*** | ***-0.46*** | ***-0.52*** | ***-0.65*** | ***-0.56*** |

[a] Optimization of *aa* form in $Me_2CO$ and $H_2O$ converged into *ag* form.

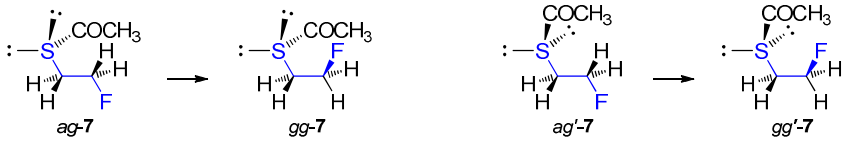
**Table S12.** Contribution of various energy components to the total binding interactions between two $FCH_2\cdot$ and $\cdot CH_2SCN$ fragments and energy changes (ΔΔE values, in bold) occuring upon conformational isomerization.[a] Values are in kcal/mol.




| conformation | $\Delta E_{tot}$ **$\Delta E_{iso}$** | $\Delta E_{def}$ **$\Delta\Delta E_{def}$** | $\Delta E_{int}$ **$\Delta\Delta E_{int}$** | $\Delta E_{elstat}$ **$\Delta\Delta E_{elstat}$** | $\Delta E_{ex+rep}$ **$\Delta\Delta E_{ex+rep}$** | $\Delta E_{oi}$ **$\Delta\Delta E_{oi}$** | $\Delta E_{disp}$ **$\Delta\Delta E_{disp}$** |
|---|---|---|---|---|---|---|---|
| *aa*-**6** | -94.74 | 17.18 | -111.92 | -144.12 | 217.87 | -154.09 | -31.58 |
| *ag/g′*-**6** | -97.25 | 12.69 | -109.94 | -148.73 | 225.88 | -156.93 | -30.16 |
| *ga*-**6** | -95.75 | 17.91 | -113.66 | -146.52 | 220.74 | -156.06 | -31.82 |
| *gg*-**6** | -97.09 | 13.23 | -110.32 | -149.34 | 226.88 | -157.78 | -30.08 |
| *gg′*-**6** | -95.60 | 12.72 | -108.32 | -148.87 | 229.07 | -158.34 | -30.18 |
| *aa*-**6** → *ga*-**6** | **-1.01** | **0.73** | **-1.74** | **-2.40** | **2.87** | **-1.97** | **-0.24** |
| *ag*-**6** → *gg*-**6** | **0.16** | **0.54** | **-0.38** | **-0.61** (42%) | **1.00** | **-0.85** (58%) | **0.08** |
| *ag′*-**6** → *gg′*-**6** | **1.66** | **0.04** | **1.62** | **-0.14** | **3.19** | **-1.41** | **-0.02** |

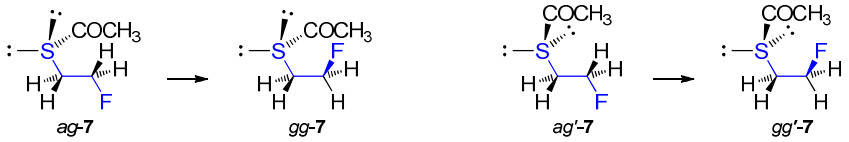
[a] Labeling of various energy terms is the same as in Table S2. Values in parentheses are percentage contribution to all attractive interactions.

**Table S13.** Calculated relative electronic energies ΔE, enthalpies ΔH and free energies ΔG of three conformers of **7** and energy changes (in bold) occuring upon conformational isomerization (MP2/6-311++G(d,p) regular, B3LYP/6-311++G(d,p) italic). Values are in kcal/mol.




| conformation | gas-phase | | | in $CH_2Cl_2$ | | | in $Me_2CO$ | | | in $H_2O$ | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | ΔE | ΔH | ΔG | ΔE | ΔH | ΔG | ΔE | ΔH | ΔG | ΔE | ΔH | ΔG |
| *ag/g′*-**7** | 0.00 | 0.00 | 0.00 | 0.00 | 0.05 | 0.08 | 0.00 | 0.06 | 0.10 | 0.00 | 0.06 | 0.11 |
| | *0.00* | *0.03* | *0.27* | *0.15* | *0.24* | *0.15* | *0.16* | *0.25* | *0.00* | *0.17* | *0.25* | *0.00* |
| *gg*-**7** | 0.22 | 0.11 | 0.12 | 0.05 | 0.00 | 0.00 | 0.05 | 0.00 | 0.00 | 0.04 | 0.00 | 0.00 |
| | *0.07* | *0.00* | *0.00* | *0.00* | *0.00* | *0.00* | *0.00* | *0.00* | *0.35* | *0.00* | *0.00* | *0.02* |
| *gg′*-**7** | 1.45 | 1.34 | 1.32 | 0.78 | 0.70 | 0.60 | 0.66 | 0.59 | 0.52 | 0.58 | 0.51 | 0.47 |
| | *1.21* | *1.11* | *1.40* | *0.55* | *0.53* | *1.07* | *0.42* | *0.40* | *1.21* | *0.33* | *0.31* | *0.75* |
| *ag*-**7** → *gg*-**7** | **0.22** | **0.11** | **0.12** | **0.05** | **-0.05** | **-0.08** | **0.05** | **-0.06** | **-0.10** | **0.04** | **-0.06** | **-0.11** |
| | ***0.07*** | ***-0.03*** | ***-0.27*** | ***-0.15*** | ***-0.24*** | ***-0.15*** | ***-0.16*** | ***-0.25*** | ***0.35*** | ***-0.17*** | ***-0.25*** | ***0.02*** |
| *ag′*-**7** → *gg′*-**7** | **1.45** | **1.34** | **1.32** | **0.78** | **0.65** | **0.52** | **0.66** | **0.53** | **0.42** | **0.58** | **0.45** | **0.36** |
| | ***1.21*** | ***1.08*** | ***1.13*** | ***0.40*** | ***0.29*** | ***0.92*** | ***0.26*** | ***0.15*** | ***1.21*** | ***0.17*** | ***0.06*** | ***0.75*** |

**Table S14.** Contribution of various energy components to the total binding interactions between two $FCH_2$· and ·$CH_2SCOCH_3$ fragments and energy changes (ΔΔE values, in bold) occuring upon conformational isomerization.[a] Values are in kcal/mol.




| conformation | $\Delta E_{tot}$ **$\Delta E_{iso}$** | $\Delta E_{def}$ **$\Delta\Delta E_{def}$** | $\Delta E_{int}$ **$\Delta\Delta E_{int}$** | $\Delta E_{elstat}$ **$\Delta\Delta E_{elstat}$** | $\Delta E_{ex+rep}$ **$\Delta\Delta E_{ex+rep}$** | $\Delta E_{oi}$ **$\Delta\Delta E_{oi}$** | $\Delta E_{disp}$ **$\Delta\Delta E_{disp}$** |
|---|---|---|---|---|---|---|---|
| *ag/g′*-**7** | -96.34 | 13.39 | -109.73 | -151.70 | 229.01 | -157.14 | -29.90 |
| *gg*-**7** | -96.12 | 13.97 | -110.09 | -152.33 | 229.45 | -157.67 | -29.54 |
| *gg′*-**7** | -94.91 | 13.71 | -108.63 | -151.23 | 229.95 | -157.38 | -29.96 |
| *ag*-**7** → *gg*-**7** | **0.22** | **0.58** | **-0.36** | **-0.63** (54%) | **0.44** | **-0.53** (46%) | **0.36** |
| *ag′*-**7** → *gg′*-**7** | **1.45** | **0.34** | **1.11** | **0.47** | **0.94** | **-0.24** | **-0.06** |

[a] Labeling of various energy terms is the same as in Table S2. Values in parentheses are percentage contribution to all attractive interactions.

## Second-order perturbation analysis of donor-acceptor interactions

The second-order perturbation analysis in NBO basis allows us to quantify stabilizing energy, denoted as E(2), due to charge transfer between an occupied and an empty orbital, as expressed in Eq. 1. In the equation, $q_i$ represents occupancy of donor orbital (~2), $F_{i,j}$ is Fock matrix element between interacting orbitals related to the amount of their overlap and $\Delta E_{i,j}$ is energy difference between the orbitals (for more details, see ref. 35 in the manuscript).

$$E(2) = -q_i(F_{i,j})^2/\Delta E_{i,j} \qquad (1)$$

The interacting orbital energies, their energy difference and Fock matrix element for selected *gauche* conformers of **1** and **3-5** are listed in Table S15. Calculated E(2) values are presented in Table 8, in the manuscript.

**Table S15.** Orbital energies (E), difference in energy (ΔE) and Fock matrix element (F) between interacting orbtals (HF/6-311++G(d,p)). Values are in a.u.

| conformation | $E_{C–H}$ | $E_{C–F}^*$ | $E_{C–H}$ | $E_{C–S}^*$ | $\Delta E_{CH/CF}^*$ | $\Delta E_{CH/CS}^*$ | $F_{CH/CF}^*$ | $F_{CH/CS}^*$ |
|---|---|---|---|---|---|---|---|---|
| *gg′*-**1** | -0.714 | 0.483 | -0.724 | 0.370 | 1.20 | 1.09 | 0.075 | 0.073 |
| *g′a*-**3** | -0.734 | 0.484 | -0.728 | 0.332 | 1.22 | 1.06 | 0.072 | 0.063 |
| *g′g*-**3** | -0.727 | 0.463 | -0.741 | 0.334 | 1.19 | 1.08 | 0.077 | 0.067 |
| *gg′*-**3** | -0.729 | 0.479 | -0.728 | 0.332 | 1.21 | 1.06 | 0.072 | 0.066 |
| *gg′*-**4** | -0.745 | 0.462 | -0.745 | 0.321 | 1.21 | 1.07 | 0.073 | 0.068 |
| *ga*-**5** | -0.905 | 0.331 | -0.882 | 0.153 | 1.24 | 1.03 | 0.070 | 0.077 |
| *gg*-**5** | -0.910 | 0.337 | -0.878 | 0.150 | 1.25 | 1.03 | 0.068 | 0.070 |
| *gg′*-**5** | -0.914 | 0.342 | -0.879 | 0.151 | 1.26 | 1.03 | 0.065 | 0.070 |

## Absolute energies (a.u.) and x, y, z coordinates (Å) of optimized structures at the MP2/6-311++G(d,p) level

***ag*-1**

E = -576.4893691 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.018838 | 0.611892 | 0.076135 |
| 2 | 1 | 0 | 0.106287 | 1.139073 | 1.023471 |
| 3 | 1 | 0 | 0.092436 | 1.334559 | -0.735337 |
| 4 | 6 | 0 | 1.022845 | -0.478713 | -0.065489 |
| 5 | 1 | 0 | 0.938531 | -1.215116 | 0.738655 |
| 6 | 1 | 0 | 0.933300 | -0.982771 | -1.030188 |
| 7 | 9 | 0 | 2.297026 | 0.085138 | 0.012793 |
| 8 | 16 | 0 | -1.696639 | -0.062241 | -0.073854 |
| 9 | 1 | 0 | -1.621594 | -0.845200 | 1.006055 |

***ga*-1**

E = -576.4860491 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.075999 | 0.872884 | -0.280907 |
| 2 | 1 | 0 | -0.347858 | 1.835553 | 0.160243 |
| 3 | 1 | 0 | 0.059797 | 0.997003 | -1.357461 |
| 4 | 6 | 0 | 1.228509 | 0.435335 | 0.346586 |
| 5 | 1 | 0 | 2.015213 | 1.167441 | 0.142475 |
| 6 | 1 | 0 | 1.122739 | 0.290477 | 1.424491 |
| 7 | 9 | 0 | 1.634373 | -0.779347 | -0.202272 |
| 8 | 16 | 0 | -1.380213 | -0.352605 | 0.066120 |
| 9 | 1 | 0 | -2.390900 | 0.516022 | -0.001305 |

***gg*-1**

E = -576.4867784 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.071439 | 0.835487 | -0.312012 |
| 2 | 1 | 0 | -0.326694 | 1.850468 | 0.006163 |
| 3 | 1 | 0 | 0.073209 | 0.850059 | -1.395191 |
| 4 | 6 | 0 | 1.225143 | 0.422132 | 0.352840 |
| 5 | 1 | 0 | 1.997680 | 1.176974 | 0.173600 |
| 6 | 1 | 0 | 1.097630 | 0.279165 | 1.429686 |
| 7 | 9 | 0 | 1.681808 | -0.776232 | -0.180468 |
| 8 | 16 | 0 | -1.459893 | -0.291926 | -0.008569 |
| 9 | 1 | 0 | -1.542044 | -0.045479 | 1.302085 |

***gg′*-1**

E = -576.4896925 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.075521 | 0.862261 | -0.315586 |
| 2 | 1 | 0 | -0.349390 | 1.855535 | 0.052373 |
| 3 | 1 | 0 | 0.057457 | 0.925024 | -1.398162 |
| 4 | 6 | 0 | 1.223255 | 0.446832 | 0.337968 |
| 5 | 1 | 0 | 2.019072 | 1.162050 | 0.109392 |
| 6 | 1 | 0 | 1.107884 | 0.340329 | 1.418882 |
| 7 | 9 | 0 | 1.623742 | -0.792372 | -0.164403 |
| 8 | 16 | 0 | -1.465417 | -0.229088 | 0.095547 |
| 9 | 1 | 0 | -0.888426 | -1.340728 | -0.365894 |

***aa*-2**

E = -615.699038 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.345721 | 0.427416 | -0.110240 |
| 2 | 1 | 0 | 0.282079 | 1.180775 | 0.680550 |
| 3 | 1 | 0 | 0.412859 | 0.928238 | -1.080085 |
| 4 | 6 | 0 | 1.587560 | -0.414794 | 0.108205 |
| 5 | 1 | 0 | 1.598846 | -0.854061 | 1.108159 |
| 6 | 1 | 0 | 1.671583 | -1.205679 | -0.641794 |
| 7 | 9 | 0 | 2.713740 | 0.400462 | -0.010188 |
| 8 | 16 | 0 | -1.115060 | -0.644066 | -0.045092 |
| 9 | 6 | 0 | -2.369456 | 0.647480 | 0.076380 |
| 10 | 1 | 0 | -2.254118 | 1.226553 | 0.995320 |
| 11 | 1 | 0 | -3.342505 | 0.152705 | 0.095003 |
| 12 | 1 | 0 | -2.334395 | 1.311763 | -0.790052 |

*ag*-**2**

E = -615.700953 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.398637 | -0.549319 | 0.479670 |
| 2 | 1 | 0 | -0.388066 | -0.103508 | 1.478949 |
| 3 | 1 | 0 | -0.754372 | -1.578982 | 0.571466 |
| 4 | 6 | 0 | -1.324717 | 0.225134 | -0.436639 |
| 5 | 1 | 0 | -0.999811 | 1.260696 | -0.560481 |
| 6 | 1 | 0 | -1.394226 | -0.254900 | -1.415304 |
| 7 | 9 | 0 | -2.606284 | 0.256189 | 0.119866 |
| 8 | 16 | 0 | 1.282773 | -0.639106 | -0.178598 |
| 9 | 6 | 0 | 1.821049 | 1.057512 | 0.138213 |
| 10 | 1 | 0 | 1.335703 | 1.783900 | -0.515216 |
| 11 | 1 | 0 | 2.895791 | 1.088420 | -0.052479 |
| 12 | 1 | 0 | 1.651004 | 1.324412 | 1.184369 |

*ga*-**2**

E = -615.6981916 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.278608 | 0.788116 | 0.146086 |
| 2 | 1 | 0 | 0.078197 | 1.676408 | -0.388867 |
| 3 | 1 | 0 | -0.311047 | 1.007602 | 1.218030 |
| 4 | 6 | 0 | -1.677744 | 0.490632 | -0.348688 |
| 5 | 1 | 0 | -2.326345 | 1.357306 | -0.191589 |
| 6 | 1 | 0 | -1.675877 | 0.217333 | -1.407123 |
| 7 | 9 | 0 | -2.223563 | -0.575466 | 0.361919 |
| 8 | 16 | 0 | 0.841276 | -0.595514 | -0.187500 |
| 9 | 6 | 0 | 2.391957 | 0.256556 | 0.168095 |
| 10 | 1 | 0 | 2.559515 | 1.089321 | -0.519492 |
| 11 | 1 | 0 | 3.197811 | -0.468868 | 0.039188 |
| 12 | 1 | 0 | 2.415765 | 0.616489 | 1.199623 |

***gg*-2**

E = -615.6988463 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.368432 | -0.300973 | 0.908616 |
| 2 | 1 | 0 | 0.014777 | 0.169838 | 1.822090 |
| 3 | 1 | 0 | -0.830690 | -1.251396 | 1.190343 |
| 4 | 6 | 0 | -1.429327 | 0.591663 | 0.296832 |
| 5 | 1 | 0 | -2.183097 | 0.851476 | 1.047263 |
| 6 | 1 | 0 | -1.005302 | 1.508348 | -0.121275 |
| 7 | 9 | 0 | -2.081200 | -0.077714 | -0.732873 |
| 8 | 16 | 0 | 1.011125 | -0.704754 | -0.187457 |
| 9 | 6 | 0 | 1.860330 | 0.888570 | -0.172189 |
| 10 | 1 | 0 | 1.281039 | 1.673683 | -0.662415 |
| 11 | 1 | 0 | 2.790606 | 0.757024 | -0.728849 |
| 12 | 1 | 0 | 2.110046 | 1.190952 | 0.848461 |

***gg′*-2**

E = -615.7006776 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.408114 | -0.912725 | 0.532066 |
| 2 | 1 | 0 | 0.507045 | -2.003746 | 0.556593 |
| 3 | 1 | 0 | 0.376003 | -0.558575 | 1.568021 |
| 4 | 6 | 0 | 1.626205 | -0.352511 | -0.171424 |
| 5 | 1 | 0 | 2.544999 | -0.697347 | 0.314108 |
| 6 | 1 | 0 | 1.632761 | -0.630816 | -1.227916 |
| 7 | 9 | 0 | 1.623928 | 1.042243 | -0.106317 |
| 8 | 16 | 0 | -1.169758 | -0.576726 | -0.284319 |
| 9 | 6 | 0 | -1.435662 | 1.143632 | 0.204353 |
| 10 | 1 | 0 | -1.392665 | 1.245145 | 1.291556 |
| 11 | 1 | 0 | -2.442929 | 1.406185 | -0.126369 |
| 12 | 1 | 0 | -0.716382 | 1.816207 | -0.260006 |

*aa*-**3**

E = -690.7491299 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.550758 | -0.616967 | 0.044819 |
| 2 | 1 | 0 | 0.475857 | -0.909409 | 1.096668 |
| 3 | 1 | 0 | 0.675012 | -1.499255 | -0.591025 |
| 4 | 6 | 0 | 1.709833 | 0.344384 | -0.145891 |
| 5 | 1 | 0 | 1.609135 | 1.209722 | 0.509937 |
| 6 | 1 | 0 | 1.789180 | 0.675968 | -1.185046 |
| 7 | 9 | 0 | 2.891914 | -0.318436 | 0.180470 |
| 8 | 16 | 0 | -0.988588 | 0.222246 | -0.435285 |
| 9 | 6 | 0 | -2.097857 | -1.036091 | 0.233152 |
| 10 | 1 | 0 | -3.117441 | -0.701265 | 0.035633 |
| 11 | 1 | 0 | -1.914978 | -1.990151 | -0.268068 |
| 12 | 1 | 0 | -1.934681 | -1.111461 | 1.310751 |
| 13 | 8 | 0 | -1.096038 | 1.435985 | 0.454876 |

*ag*-**3**

E = -690.746465 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.574743 | -0.546567 | 0.285813 |
| 2 | 1 | 0 | -0.774101 | -1.579536 | -0.012777 |
| 3 | 1 | 0 | -0.471527 | -0.507466 | 1.374386 |
| 4 | 6 | 0 | -1.686144 | 0.349648 | -0.227563 |
| 5 | 1 | 0 | -1.665329 | 0.424250 | -1.319212 |
| 6 | 1 | 0 | -1.645013 | 1.349802 | 0.208902 |
| 7 | 9 | 0 | -2.911699 | -0.206133 | 0.131439 |
| 8 | 16 | 0 | 1.055126 | -0.169368 | -0.432831 |
| 9 | 6 | 0 | 1.215409 | 1.491232 | 0.262992 |
| 10 | 1 | 0 | 2.236167 | 1.813300 | 0.049417 |
| 11 | 1 | 0 | 0.509744 | 2.176081 | -0.214373 |
| 12 | 1 | 0 | 1.064154 | 1.446275 | 1.344635 |
| 13 | 8 | 0 | 2.042756 | -1.040439 | 0.297990 |

*ag'*-**3**

E = -690.7481091 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.612315 | 0.009139 | 0.792763 |
| 2 | 1 | 0 | 0.709923 | 0.898323 | 1.422869 |
| 3 | 1 | 0 | 0.918911 | -0.867902 | 1.369923 |
| 4 | 6 | 0 | 1.461199 | 0.092275 | -0.460925 |
| 5 | 1 | 0 | 1.312156 | 1.028578 | -1.002108 |
| 6 | 1 | 0 | 1.255882 | -0.753822 | -1.118222 |
| 7 | 9 | 0 | 2.804264 | 0.042267 | -0.084778 |
| 8 | 16 | 0 | -1.155144 | -0.251270 | 0.435196 |
| 9 | 6 | 0 | -1.481119 | 1.348542 | -0.348559 |
| 10 | 1 | 0 | -2.552209 | 1.377091 | -0.555305 |
| 11 | 1 | 0 | -1.215189 | 2.160522 | 0.333058 |
| 12 | 1 | 0 | -0.933263 | 1.416935 | -1.289893 |
| 13 | 8 | 0 | -1.225831 | -1.289944 | -0.657515 |

*ga*-**3**

E = -690.7449424 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.459094 | -0.850585 | 0.425647 |
| 2 | 1 | 0 | 0.433641 | -0.573525 | 1.484916 |
| 3 | 1 | 0 | 0.145034 | -1.892857 | 0.299507 |
| 4 | 6 | 0 | 1.848213 | -0.691361 | -0.155853 |
| 5 | 1 | 0 | 1.851428 | -0.893387 | -1.231284 |
| 6 | 1 | 0 | 2.547010 | -1.370067 | 0.341790 |
| 7 | 9 | 0 | 2.303353 | 0.605227 | 0.031806 |
| 8 | 16 | 0 | -0.759392 | 0.226072 | -0.414110 |
| 9 | 6 | 0 | -2.202359 | -0.746854 | 0.082961 |
| 10 | 1 | 0 | -3.080170 | -0.177692 | -0.227303 |
| 11 | 1 | 0 | -2.192051 | -1.719050 | -0.416103 |
| 12 | 1 | 0 | -2.204000 | -0.854689 | 1.170566 |
| 13 | 8 | 0 | -0.838810 | 1.518734 | 0.350111 |

***gg*-3**

E = -690.7476138 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.478158 | -0.806732 | 0.582166 |
| 2 | 1 | 0 | -0.605591 | -1.827497 | 0.211789 |
| 3 | 1 | 0 | -0.077664 | -0.852239 | 1.601542 |
| 4 | 6 | 0 | -1.793427 | -0.058926 | 0.552524 |
| 5 | 1 | 0 | -1.713417 | 0.935382 | 0.997116 |
| 6 | 1 | 0 | -2.562167 | -0.626191 | 1.083836 |
| 7 | 9 | 0 | -2.218850 | 0.102547 | -0.765362 |
| 8 | 16 | 0 | 0.858112 | -0.107287 | -0.445925 |
| 9 | 6 | 0 | 0.874181 | 1.538777 | 0.301541 |
| 10 | 1 | 0 | 1.774919 | 2.024682 | -0.077854 |
| 11 | 1 | 0 | -0.004148 | 2.108765 | -0.009966 |
| 12 | 1 | 0 | 0.940093 | 1.451152 | 1.389352 |
| 13 | 8 | 0 | 2.109031 | -0.807388 | 0.026233 |

***gg′*-3**

E = -690.7512777 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.541542 | -0.673553 | 0.896259 |
| 2 | 1 | 0 | 0.813988 | -0.071567 | 1.768218 |
| 3 | 1 | 0 | 0.429312 | -1.717774 | 1.206003 |
| 4 | 6 | 0 | 1.589687 | -0.599865 | -0.191540 |
| 5 | 1 | 0 | 1.178858 | -0.949340 | -1.142420 |
| 6 | 1 | 0 | 2.467760 | -1.190466 | 0.080354 |
| 7 | 9 | 0 | 2.012335 | 0.721729 | -0.359772 |
| 8 | 16 | 0 | -1.130981 | -0.202862 | 0.324718 |
| 9 | 6 | 0 | -0.838784 | 1.557126 | 0.041840 |
| 10 | 1 | 0 | -1.800454 | 1.979703 | -0.254230 |
| 11 | 1 | 0 | -0.492121 | 2.029190 | 0.964398 |
| 12 | 1 | 0 | -0.110566 | 1.680620 | -0.759147 |
| 13 | 8 | 0 | -1.282096 | -0.839049 | -1.037508 |

*g′a*-**3**

E = -690.7507055 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.456927 | -0.818879 | 0.462439 |
| 2 | 1 | 0 | 0.056993 | -0.994078 | 1.467607 |
| 3 | 1 | 0 | 0.573426 | -1.763190 | -0.078124 |
| 4 | 6 | 0 | 1.781925 | -0.096823 | 0.570347 |
| 5 | 1 | 0 | 2.477954 | -0.663448 | 1.193660 |
| 6 | 1 | 0 | 1.644313 | 0.907514 | 0.977291 |
| 7 | 9 | 0 | 2.345422 | 0.022258 | -0.699030 |
| 8 | 16 | 0 | -0.743745 | 0.235634 | -0.415753 |
| 9 | 6 | 0 | -2.177825 | -0.802133 | -0.052746 |
| 10 | 1 | 0 | -3.046639 | -0.318076 | -0.501633 |
| 11 | 1 | 0 | -2.035698 | -1.791899 | -0.494891 |
| 12 | 1 | 0 | -2.306996 | -0.861949 | 1.030733 |
| 13 | 8 | 0 | -0.867300 | 1.477707 | 0.433554 |

*g′g*-**3**

E = -690.7494256 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.471319 | -0.846224 | 0.537074 |
| 2 | 1 | 0 | -0.217637 | -1.911524 | 0.553697 |
| 3 | 1 | 0 | -0.448826 | -0.462827 | 1.561780 |
| 4 | 6 | 0 | -1.828964 | -0.672081 | -0.107297 |
| 5 | 1 | 0 | -2.590105 | -1.223633 | 0.449814 |
| 6 | 1 | 0 | -1.823697 | -1.004800 | -1.148691 |
| 7 | 9 | 0 | -2.198595 | 0.674914 | -0.102203 |
| 8 | 16 | 0 | 0.894506 | -0.104968 | -0.423274 |
| 9 | 6 | 0 | 0.782944 | 1.560473 | 0.260553 |
| 10 | 1 | 0 | 1.568088 | 2.148610 | -0.217388 |
| 11 | 1 | 0 | -0.199696 | 1.982694 | 0.045190 |
| 12 | 1 | 0 | 0.969046 | 1.502991 | 1.336025 |
| 13 | 8 | 0 | 2.165266 | -0.709907 | 0.121225 |

*g′g′*-**3**

E = -690.7436533 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.497633 | -0.752163 | 0.707556 |
| 2 | 1 | 0 | -0.148307 | -1.782742 | 0.823790 |
| 3 | 1 | 0 | -0.983630 | -0.441101 | 1.635511 |
| 4 | 6 | 0 | -1.493001 | -0.608014 | -0.433821 |
| 5 | 1 | 0 | -2.053467 | -1.536820 | -0.570020 |
| 6 | 1 | 0 | -1.010208 | -0.320587 | -1.371008 |
| 7 | 9 | 0 | -2.407312 | 0.387519 | -0.117823 |
| 8 | 16 | 0 | 0.982695 | 0.313209 | 0.492069 |
| 9 | 6 | 0 | 1.876397 | -0.828789 | -0.592115 |
| 10 | 1 | 0 | 2.772118 | -0.300604 | -0.923028 |
| 11 | 1 | 0 | 2.157546 | -1.728963 | -0.039775 |
| 12 | 1 | 0 | 1.259891 | -1.071385 | -1.461335 |
| 13 | 8 | 0 | 0.579270 | 1.477122 | -0.374568 |

*aa*-**4**

E = -765.8415171 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.956984 | 0.262746 | 0.000000 |
| 2 | 1 | 0 | -1.286958 | 0.790033 | 0.898358 |
| 3 | 1 | 0 | -1.286958 | 0.790033 | -0.898358 |
| 4 | 6 | 0 | -1.486105 | -1.164118 | 0.000000 |
| 5 | 1 | 0 | -1.168707 | -1.701764 | 0.894716 |
| 6 | 1 | 0 | -1.168707 | -1.701764 | -0.894716 |
| 7 | 9 | 0 | -2.877048 | -1.099258 | 0.000000 |
| 8 | 16 | 0 | 0.837705 | 0.240320 | 0.000000 |
| 9 | 6 | 0 | 1.269920 | 1.969787 | 0.000000 |
| 10 | 1 | 0 | 2.361267 | 2.000163 | 0.000000 |
| 11 | 1 | 0 | 0.880257 | 2.438153 | -0.904442 |
| 12 | 1 | 0 | 0.880257 | 2.438153 | 0.904442 |
| 13 | 8 | 0 | 1.269920 | -0.338456 | 1.269406 |
| 14 | 8 | 0 | 1.269920 | -0.338456 | -1.269406 |

*ag*-**4**

E = -765.8412539 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.749902 | -0.441098 | -0.534938 |
| 2 | 1 | 0 | 0.865335 | -1.528535 | -0.527685 |
| 3 | 1 | 0 | 0.803552 | -0.089706 | -1.568593 |
| 4 | 6 | 0 | 1.803285 | 0.218541 | 0.339016 |
| 5 | 1 | 0 | 1.793193 | -0.197119 | 1.346727 |
| 6 | 1 | 0 | 1.671938 | 1.302629 | 0.388099 |
| 7 | 9 | 0 | 3.049584 | -0.027343 | -0.230311 |
| 8 | 16 | 0 | -0.919060 | -0.161853 | 0.061428 |
| 9 | 6 | 0 | -1.276135 | 1.522847 | -0.409547 |
| 10 | 1 | 0 | -2.290995 | 1.714118 | -0.055567 |
| 11 | 1 | 0 | -0.577537 | 2.201137 | 0.081579 |
| 12 | 1 | 0 | -1.234800 | 1.608987 | -1.495874 |
| 13 | 8 | 0 | -1.808367 | -1.028921 | -0.701575 |
| 14 | 8 | 0 | -0.870918 | -0.218269 | 1.520836 |

*ga*-**4**

E = -765.8393992 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.599330 | -0.880557 | -0.569509 |
| 2 | 1 | 0 | -0.691590 | -0.673130 | -1.638202 |
| 3 | 1 | 0 | -0.278770 | -1.914807 | -0.407611 |
| 4 | 6 | 0 | -1.916422 | -0.657667 | 0.149340 |
| 5 | 1 | 0 | -1.780763 | -0.698577 | 1.232193 |
| 6 | 1 | 0 | -2.637402 | -1.415396 | -0.168784 |
| 7 | 9 | 0 | -2.429704 | 0.587741 | -0.178625 |
| 8 | 16 | 0 | 0.707872 | 0.171536 | 0.098321 |
| 9 | 6 | 0 | 2.188952 | -0.645004 | -0.473969 |
| 10 | 1 | 0 | 3.018377 | -0.019248 | -0.139268 |
| 11 | 1 | 0 | 2.257874 | -1.636141 | -0.024696 |
| 12 | 1 | 0 | 2.173988 | -0.691461 | -1.563931 |
| 13 | 8 | 0 | 0.654837 | 1.480649 | -0.538770 |
| 14 | 8 | 0 | 0.650223 | 0.033587 | 1.552474 |

*gg*-**4**

E = -765.8379012 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.604211 | -1.118696 | -0.136414 |
| 2 | 1 | 0 | 0.696177 | -1.670132 | 0.803579 |
| 3 | 1 | 0 | 0.335428 | -1.811623 | -0.938865 |
| 4 | 6 | 0 | 1.903613 | -0.419956 | -0.487224 |
| 5 | 1 | 0 | 1.836982 | 0.095960 | -1.448596 |
| 6 | 1 | 0 | 2.708071 | -1.158754 | -0.536480 |
| 7 | 9 | 0 | 2.238972 | 0.519420 | 0.476713 |
| 8 | 16 | 0 | -0.831418 | -0.050571 | 0.126982 |
| 9 | 6 | 0 | -0.614510 | 1.290408 | -1.029093 |
| 10 | 1 | 0 | -1.507614 | 1.907785 | -0.914195 |
| 11 | 1 | 0 | 0.272989 | 1.862772 | -0.758988 |
| 12 | 1 | 0 | -0.566009 | 0.898370 | -2.046268 |
| 13 | 8 | 0 | -2.001654 | -0.817778 | -0.291692 |
| 14 | 8 | 0 | -0.746342 | 0.505207 | 1.470950 |

*gg′*-**4**

E = -765.8451258 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.613755 | -0.854330 | -0.685686 |
| 2 | 1 | 0 | -0.682991 | -0.505093 | -1.719107 |
| 3 | 1 | 0 | -0.362273 | -1.920284 | -0.690567 |
| 4 | 6 | 0 | -1.898701 | -0.631133 | 0.079633 |
| 5 | 1 | 0 | -1.767069 | -0.855076 | 1.139785 |
| 6 | 1 | 0 | -2.700027 | -1.242152 | -0.342667 |
| 7 | 9 | 0 | -2.283753 | 0.706540 | -0.032668 |
| 8 | 16 | 0 | 0.835260 | -0.099001 | 0.072401 |
| 9 | 6 | 0 | 0.675899 | 1.647083 | -0.243527 |
| 10 | 1 | 0 | 1.559293 | 2.102192 | 0.208557 |
| 11 | 1 | 0 | 0.675333 | 1.814707 | -1.321109 |
| 12 | 1 | 0 | -0.235119 | 2.017056 | 0.224219 |
| 13 | 8 | 0 | 0.721426 | -0.310664 | 1.514023 |
| 14 | 8 | 0 | 1.993800 | -0.583825 | -0.672277 |

*aa*-**5**

E = -655.2443329 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.771204 | -0.700661 | 0.000000 |
| 2 | 1 | 0 | -1.376593 | -0.923733 | 0.883871 |
| 3 | 1 | 0 | -1.376593 | -0.923733 | -0.883871 |
| 4 | 6 | 0 | 0.509147 | -1.531239 | 0.000000 |
| 5 | 1 | 0 | 1.110712 | -1.359166 | 0.895522 |
| 6 | 1 | 0 | 1.110712 | -1.359166 | -0.895522 |
| 7 | 9 | 0 | 0.104605 | -2.846722 | 0.000000 |
| 8 | 16 | 0 | -0.571785 | 1.096551 | 0.000000 |
| 9 | 6 | 0 | 0.509147 | 1.419929 | -1.405194 |
| 10 | 1 | 0 | 0.615085 | 2.503701 | -1.478575 |
| 11 | 1 | 0 | 1.481632 | 0.946512 | -1.273507 |
| 12 | 1 | 0 | 0.004005 | 1.046658 | -2.298009 |
| 13 | 6 | 0 | 0.509147 | 1.419929 | 1.405194 |
| 14 | 1 | 0 | 0.615085 | 2.503701 | 1.478575 |
| 15 | 1 | 0 | 0.004005 | 1.046658 | 2.298009 |
| 16 | 1 | 0 | 1.481632 | 0.946512 | 1.273507 |

*ag*-**5**

E = -655.2459725 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.632469 | -0.542400 | 0.202313 |
| 2 | 1 | 0 | 0.548124 | -0.522363 | 1.292575 |
| 3 | 1 | 0 | 0.770203 | -1.572796 | -0.138260 |
| 4 | 6 | 0 | 1.804672 | 0.313600 | -0.279412 |
| 5 | 1 | 0 | 1.737128 | 1.343333 | 0.080273 |
| 6 | 1 | 0 | 1.886494 | 0.301650 | -1.369503 |
| 7 | 9 | 0 | 2.936152 | -0.255795 | 0.256800 |
| 8 | 16 | 0 | -0.933919 | 0.006362 | -0.518831 |
| 9 | 6 | 0 | -1.255376 | 1.542256 | 0.366080 |
| 10 | 1 | 0 | -2.291176 | 1.820031 | 0.162287 |
| 11 | 1 | 0 | -1.092748 | 1.398732 | 1.435828 |
| 12 | 1 | 0 | -0.593661 | 2.310210 | -0.035556 |
| 13 | 6 | 0 | -2.095075 | -1.122557 | 0.269650 |
| 14 | 1 | 0 | -3.099898 | -0.810348 | -0.019821 |
| 15 | 1 | 0 | -1.896851 | -2.121199 | -0.122689 |
| 16 | 1 | 0 | -1.970425 | -1.092284 | 1.353178 |

*ga*-**5**

E = -655.2529122 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.699894 | -0.110462 | 1.148997 |
| 2 | 1 | 0 | 0.778071 | 0.869975 | 1.627635 |
| 3 | 1 | 0 | 0.759424 | -0.877768 | 1.926900 |
| 4 | 6 | 0 | 1.797701 | -0.315374 | 0.120803 |
| 5 | 1 | 0 | 1.770072 | -1.312529 | -0.322741 |
| 6 | 1 | 0 | 2.765314 | -0.163236 | 0.604623 |
| 7 | 9 | 0 | 1.655033 | 0.615296 | -0.898189 |
| 8 | 16 | 0 | -1.008778 | -0.176732 | 0.519585 |
| 9 | 6 | 0 | -0.938530 | -1.301337 | -0.884429 |
| 10 | 1 | 0 | -1.946816 | -1.332530 | -1.301617 |
| 11 | 1 | 0 | -0.222379 | -0.947366 | -1.625804 |
| 12 | 1 | 0 | -0.677784 | -2.292289 | -0.509114 |
| 13 | 6 | 0 | -1.237851 | 1.422120 | -0.281472 |
| 14 | 1 | 0 | -2.229237 | 1.399324 | -0.737761 |
| 15 | 1 | 0 | -1.221446 | 2.179378 | 0.504086 |
| 16 | 1 | 0 | -0.457355 | 1.597410 | -1.019267 |

*gg*-**5**

E = -655.2539454 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.505401 | -0.931264 | 0.477126 |
| 2 | 1 | 0 | 0.428347 | -0.617510 | 1.521925 |
| 3 | 1 | 0 | 0.225842 | -1.985480 | 0.383613 |
| 4 | 6 | 0 | 1.901149 | -0.707435 | -0.080696 |
| 5 | 1 | 0 | 1.984351 | -1.040291 | -1.117562 |
| 6 | 1 | 0 | 2.630370 | -1.231346 | 0.540481 |
| 7 | 9 | 0 | 2.171861 | 0.653315 | -0.040663 |
| 8 | 16 | 0 | -0.720234 | -0.000669 | -0.491440 |
| 9 | 6 | 0 | -0.721833 | 1.622699 | 0.291441 |
| 10 | 1 | 0 | -1.527488 | 2.195819 | -0.170892 |
| 11 | 1 | 0 | -0.882142 | 1.516281 | 1.365703 |
| 12 | 1 | 0 | 0.240639 | 2.087004 | 0.080112 |
| 13 | 6 | 0 | -2.258852 | -0.699789 | 0.131970 |
| 14 | 1 | 0 | -3.074584 | -0.087341 | -0.255991 |
| 15 | 1 | 0 | -2.346576 | -1.713740 | -0.260679 |
| 16 | 1 | 0 | -2.256968 | -0.697793 | 1.223247 |

*gg′*-**5**

E = -655.2513376 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.505471 | -0.923111 | 0.499036 |
| 2 | 1 | 0 | -0.600081 | -1.878837 | -0.023326 |
| 3 | 1 | 0 | -0.095751 | -1.081251 | 1.501476 |
| 4 | 6 | 0 | -1.847813 | -0.207563 | 0.559170 |
| 5 | 1 | 0 | -1.807539 | 0.692512 | 1.176351 |
| 6 | 1 | 0 | -2.600784 | -0.888809 | 0.960815 |
| 7 | 9 | 0 | -2.207234 | 0.161739 | -0.724783 |
| 8 | 16 | 0 | 0.687686 | 0.031167 | -0.484744 |
| 9 | 6 | 0 | 2.234096 | -0.755970 | -0.001726 |
| 10 | 1 | 0 | 3.041140 | -0.236129 | -0.520624 |
| 11 | 1 | 0 | 2.366888 | -0.705007 | 1.080040 |
| 12 | 1 | 0 | 2.193170 | -1.791520 | -0.344002 |
| 13 | 6 | 0 | 0.779025 | 1.591833 | 0.406186 |
| 14 | 1 | 0 | 1.651243 | 2.124358 | 0.022169 |
| 15 | 1 | 0 | -0.119533 | 2.163363 | 0.170791 |
| 16 | 1 | 0 | 0.874348 | 1.415864 | 1.479272 |

*aa*-**6**

E = -668.5481888 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.575542 | -0.351595 | 0.280514 |
| 2 | 1 | 0 | 0.684440 | -0.595017 | 1.338280 |
| 3 | 1 | 0 | 0.333220 | -1.251860 | -0.285576 |
| 4 | 6 | 0 | 1.855701 | 0.268526 | -0.253801 |
| 5 | 1 | 0 | 1.801385 | 0.415908 | -1.334606 |
| 6 | 1 | 0 | 2.078004 | 1.220688 | 0.236755 |
| 7 | 9 | 0 | 2.904588 | -0.602169 | 0.013175 |
| 8 | 16 | 0 | -0.768293 | 0.871362 | 0.061389 |
| 9 | 6 | 0 | -2.066134 | -0.207955 | -0.050099 |
| 10 | 7 | 0 | -2.990902 | -0.937978 | -0.130763 |

*ag*-**6**

E = -668.5522526 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.682767 | -0.638172 | 0.488005 |
| 2 | 1 | 0 | -1.210328 | -1.595474 | 0.513134 |
| 3 | 1 | 0 | -0.607225 | -0.249609 | 1.505025 |
| 4 | 6 | 0 | -1.406293 | 0.336627 | -0.422075 |
| 5 | 1 | 0 | -0.885722 | 1.295828 | -0.469056 |
| 6 | 1 | 0 | -1.516969 | -0.074451 | -1.428199 |
| 7 | 9 | 0 | -2.677288 | 0.560107 | 0.098580 |
| 8 | 16 | 0 | 0.975338 | -1.035488 | -0.149920 |
| 9 | 6 | 0 | 1.671687 | 0.500979 | 0.018940 |
| 10 | 7 | 0 | 2.173524 | 1.564850 | 0.125910 |

*ga*-**6**

E = -668.549777 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.490336 | 0.784600 | -0.230573 |
| 2 | 1 | 0 | 0.539029 | 0.962172 | -1.306410 |
| 3 | 1 | 0 | 0.004757 | 1.629026 | 0.264623 |
| 4 | 6 | 0 | 1.879264 | 0.615250 | 0.344630 |
| 5 | 1 | 0 | 2.476673 | 1.508464 | 0.143155 |
| 6 | 1 | 0 | 1.846809 | 0.422807 | 1.419691 |
| 7 | 9 | 0 | 2.507168 | -0.468578 | -0.261682 |
| 8 | 16 | 0 | -0.486328 | -0.729717 | 0.094786 |
| 9 | 6 | 0 | -2.023518 | -0.026499 | 0.003487 |
| 10 | 7 | 0 | -3.103862 | 0.447157 | -0.055394 |

*gg*-**6**

E = -668.5519936 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.677303 | -0.509638 | 0.872398 |
| 2 | 1 | 0 | -1.354119 | -1.366506 | 0.930882 |
| 3 | 1 | 0 | -0.252463 | -0.326892 | 1.862840 |
| 4 | 6 | 0 | -1.436105 | 0.708980 | 0.392282 |
| 5 | 1 | 0 | -2.173351 | 1.002293 | 1.145711 |
| 6 | 1 | 0 | -0.765781 | 1.547374 | 0.186630 |
| 7 | 9 | 0 | -2.120894 | 0.405522 | -0.776366 |
| 8 | 16 | 0 | 0.647652 | -1.042186 | -0.262644 |
| 9 | 6 | 0 | 1.632020 | 0.325899 | -0.099142 |
| 10 | 7 | 0 | 2.308522 | 1.288223 | 0.010045 |

*gg′*-**6**

E = -668.5496034 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.869461 | -0.797296 | 0.612947 |
| 2 | 1 | 0 | 0.647481 | -0.410287 | 1.609659 |
| 3 | 1 | 0 | 1.324581 | -1.787719 | 0.719316 |
| 4 | 6 | 0 | 1.828698 | 0.111116 | -0.126199 |
| 5 | 1 | 0 | 2.781003 | 0.160394 | 0.411430 |
| 6 | 1 | 0 | 1.995332 | -0.237970 | -1.148311 |
| 7 | 9 | 0 | 1.308357 | 1.394403 | -0.192998 |
| 8 | 16 | 0 | -0.689277 | -1.106418 | -0.278149 |
| 9 | 6 | 0 | -1.484768 | 0.359862 | 0.021113 |
| 10 | 7 | 0 | -2.110791 | 1.340936 | 0.221159 |

*ag*-**7**

E = -728.8382423 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.092436 | -0.519788 | -0.578192 |
| 2 | 1 | 0 | 0.937602 | 0.188284 | -1.394712 |
| 3 | 1 | 0 | 1.654160 | -1.380740 | -0.947727 |
| 4 | 6 | 0 | 1.832035 | 0.142858 | 0.568308 |
| 5 | 1 | 0 | 1.991026 | -0.558026 | 1.391574 |
| 6 | 1 | 0 | 1.292665 | 1.022990 | 0.922917 |
| 7 | 9 | 0 | 3.083813 | 0.560398 | 0.115513 |
| 8 | 16 | 0 | -0.515742 | -1.138505 | -0.033514 |
| 9 | 6 | 0 | -1.435985 | 0.392623 | -0.098370 |
| 10 | 8 | 0 | -0.946455 | 1.435541 | -0.480200 |
| 11 | 6 | 0 | -2.856947 | 0.263055 | 0.401136 |
| 12 | 1 | 0 | -3.232149 | -0.757565 | 0.303704 |
| 13 | 1 | 0 | -2.872244 | 0.543910 | 1.458801 |
| 14 | 1 | 0 | -3.491100 | 0.956834 | -0.153635 |

*gg*-**7**

E = -728.8379098 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.104885 | 0.057201 | -0.938872 |
| 2 | 1 | 0 | 0.676052 | 0.836775 | -1.574247 |
| 3 | 1 | 0 | 1.754469 | -0.581401 | -1.542418 |
| 4 | 6 | 0 | 1.904059 | 0.697614 | 0.176175 |
| 5 | 1 | 0 | 1.261177 | 1.250645 | 0.863140 |
| 6 | 1 | 0 | 2.662479 | 1.366895 | -0.241350 |
| 7 | 9 | 0 | 2.569360 | -0.286512 | 0.904008 |
| 8 | 16 | 0 | -0.242501 | -0.991830 | -0.344661 |
| 9 | 6 | 0 | -1.432687 | 0.285856 | 0.002010 |
| 10 | 8 | 0 | -1.214798 | 1.463841 | -0.208450 |
| 11 | 6 | 0 | -2.712256 | -0.227897 | 0.622718 |
| 12 | 1 | 0 | -2.881795 | -1.282683 | 0.397974 |
| 13 | 1 | 0 | -2.635460 | -0.106738 | 1.707673 |
| 14 | 1 | 0 | -3.546750 | 0.377025 | 0.263141 |

*gg'*-**7**

E = -728.835892 a.u.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.230368 | 0.628081 | 0.720028 |
| 2 | 1 | 0 | -1.674554 | 1.522254 | 1.166619 |
| 3 | 1 | 0 | -0.908833 | -0.047445 | 1.517593 |
| 4 | 6 | 0 | -2.253894 | -0.053499 | -0.165872 |
| 5 | 1 | 0 | -2.544519 | 0.582271 | -1.006470 |
| 6 | 1 | 0 | -3.138793 | -0.321373 | 0.419808 |
| 7 | 9 | 0 | -1.724573 | -1.226479 | -0.690857 |
| 8 | 16 | 0 | 0.249122 | 1.134769 | -0.184408 |
| 9 | 6 | 0 | 1.327686 | -0.240763 | 0.220174 |
| 10 | 8 | 0 | 1.039550 | -1.097076 | 1.026701 |
| 11 | 6 | 0 | 2.612352 | -0.226510 | -0.575594 |
| 12 | 1 | 0 | 2.444761 | -0.798186 | -1.493620 |
| 13 | 1 | 0 | 2.908099 | 0.789057 | -0.847444 |
| 14 | 1 | 0 | 3.398002 | -0.711827 | 0.005725 |